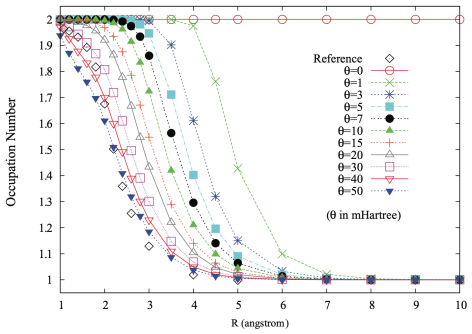
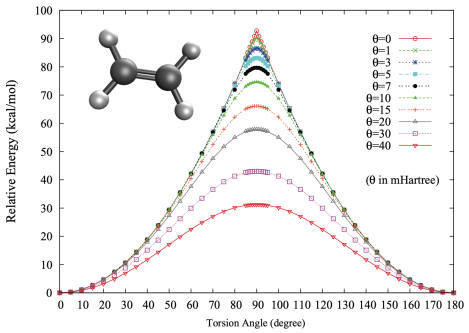
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Thermally-Assisted-Occupation Density Functional Theory (TAO-DFT)

The thermally-assisted-occuptation DFT (TAO-DFT) method, now available in Q-Chem, provides accurate descriptions of the ground states of strongly correlated systems. It uses partial orbital occupations, which are defined by a Fermi-Dirac distribution and controlled by a fictitious temperature θ, to account for multireference character.

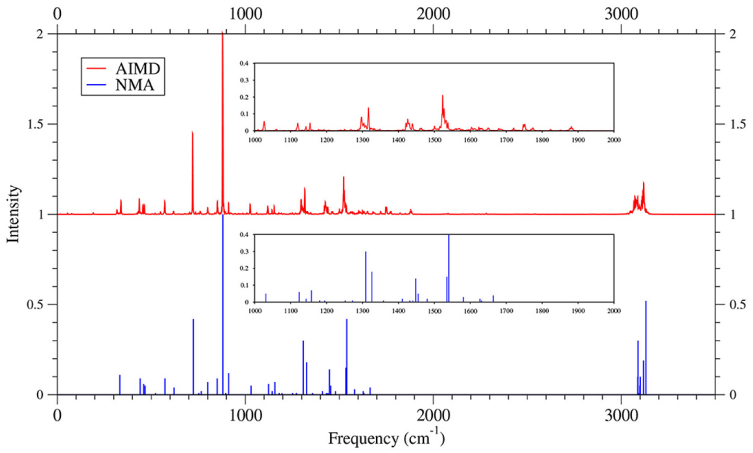


(a) Occupation numbers of the $3\sigma_g$ orbital for N_2 compared to MRCI values.



(b) Potential energy surface for the torision of twisted ethylene.

- Improved DFT description of the ground states of strongly correlated systems
- Similar computational cost to traditional KS-DFT for energies and analytical nuclear gradients
- No pre-determined active space required
- Can be used with existing XC functionals (e.g. LDA or GGA)
- Allows simulation of very large, strongly correlated polyradical systems on the nanoscale
- Can be combined with *ab initio* molecular dynamics approaches (TAO-AIMD)



Infrared spectra of 8-acene predicted using TAO-AIMD.

Request a free trial at www.q-chem.com